Short communication

An explicit algebraic reduced order algorithm for lithium ion cell voltage prediction

V. Senthil Kumar [a], Priya Gambhire [a,*], Krishnan S. Hariharan [a], Ashish Khandelwal [a], Subramanya Mayya Kolake [a], Dukjin Oh [b], Seokgwang Doo [b]

[a] Computational Simulations Group, SAIT-India Lab, TRIDIB — Bagmane Tech Park, Bangalore 560 093, India
[b] Energy Storage Group, Samsung Advanced Institute of Technology, 449712, South Korea

HIGHLIGHTS

- Earlier work reduced the 10 PDEs to 5 linear ODEs and nonlinear expressions.
- Exact solutions are derived here for a linearly varying current period.
- Explicit algebraic algorithm which can model any charge—rest—discharge protocol.

ABSTRACT

The detailed isothermal electrochemical model for a lithium ion cell has ten coupled partial differential equations to describe the cell behavior. In an earlier publication [Journal of Power Sources, 222, 426 (2013)], a reduced order model (ROM) was developed by reducing the detailed model to a set of five linear ordinary differential equations and nonlinear algebraic expressions, using uniform reaction rate, volume averaging and profile based approximations. An arbitrary current profile, involving charge, rest and discharge, is broken down into constant current and linearly varying current periods. The linearly varying current period results are generic, since it includes the constant current period results as well. Hence, the linear ordinary differential equations in ROM are solved for a linearly varying current period and an explicit algebraic algorithm is developed for lithium ion cell voltage prediction. While the existing battery management system (BMS) algorithms are equivalent circuit based and ordinary differential equations, the proposed algorithm is an explicit algebraic algorithm. These results are useful to develop a BMS algorithm for on-board applications in electric or hybrid vehicles, smart phones etc. This algorithm is simple enough for a spread-sheet implementation and is useful for rapid analysis of laboratory data.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

An isothermal model for lithium ion cell has ten coupled partial differential equations (PDEs) to describe the cell behavior [1–4], namely: two solid diffusion equations and two solid current equations in the electrode regions; three electrolyte diffusion equations and three total current balances in the negative electrode, separator and positive electrode regions, respectively. Recently, a reduced order model (ROM) has been developed [4], wherein, using uniform reaction rate, volume averaging and profile based approximations, the aforementioned ten coupled PDEs are reduced to a set of five linear ordinary differential equations (ODEs) and nonlinear algebraic expressions. The nonlinearity of the system once relegated to algebraic expressions is not computationally cumbersome. This ROM [4] shows negligible errors in cell voltage prediction at nominal currents and less than 3% error at high currents for a commercial cell.

The current work derives analytical solutions for the five linear ODEs in the ROM [4], thereby developing an algebraic algorithm for cell voltage prediction in the non-phase change lithium ion cells. Any arbitrary current profile, involving charge, rest and discharge, can be expressed as a series of constant current and linearly varying current periods. The latter is more generic, since it includes the constant current period as well. Hence, analytical solutions are derived for a linearly varying current period and the results are developed into an explicit algebraic algorithm for cell voltage prediction. This algorithm is simple enough for a spread-sheet

* Corresponding author. Tel.: +91 80 4181 9999; fax: +91 80 4181 9000.
E-mail addresses: p.gambhire@samsung.com, priya.gambhire@gmail.com
(P. Gambhire).

implementation and can be used in battery testing equipment for rapid analysis of laboratory data. It can also be easily developed into a battery management system algorithm for on-board applications in electric or hybrid vehicles and smart phones.

2. Derivation of the algebraic ROM

2.1. Solid phase Li concentration and state of charge in the electrodes

The evolution of average solid phase Li concentration in the negative electrode (Eq. (127) in Ref. [4]) is

$$\frac{d\bar{c}_{1n}}{dt} = -\frac{3\langle j_n \rangle}{r_n}. \tag{1}$$

The average reaction rate in the above equation is related to the external current and the electrode design parameters as (Eq. (14) in Ref. [4])

$$\langle j_n \rangle(t) = \frac{I(t)}{a_n F l_n}, \tag{2}$$

where, a_n is the specific surface area of the active material in negative electrode given by,

$$a_n = \frac{3\varepsilon_{1n}}{r_n}. \tag{3}$$

Using Eqs. (2) and (3) in (1) gives

$$\frac{d\bar{c}_{1n}}{dt} = -\frac{I(t)}{l_n \varepsilon_{1n} F}. \tag{4}$$

Defining the scaled average solid Li concentration in negative electrode as

$$\bar{C}_{1n} = \frac{\bar{c}_{1n}}{c_{sn\,max}}, \tag{5}$$

and the maximum specific moles of solid phase Li in the negative electrode as

$$N_{1n} = l_n \varepsilon_{1n} c_{sn\,max}, \tag{6}$$

Eq. (4) is rewritten in terms of scaled quantities as

$$\frac{d\bar{C}_{1n}}{dt} = -\frac{I(t)}{F N_{1n}}. \tag{7}$$

Time is left unscaled since there are many different time scales in this problem. Consider a linear change of external current from I_i to I_f, in the time interval t_i to t_f. The current at any time in this interval is

$$I(t) = I_i + \frac{\left(I_f - I_i\right)}{\left(t_f - t_i\right)}(t - t_i). \tag{8}$$

Using the above expression in Eq. (7) and integrating from t_i to t gives

$$\bar{C}_{1n}(t) - \bar{C}_{1n}(t_i) = -\frac{1}{F N_{1n}}\left[I_i \int_{t_i}^{t} dt + \frac{\left(I_f - I_i\right)}{\left(t_f - t_i\right)}\int_{t_i}^{t}(t - t_i)dt\right]. \tag{9}$$

On integrating and rearranging the above expression, the scaled average concentration of solid phase Li in the negative electrode at any time is

$$\bar{C}_{1n}(t) = \bar{C}_{1n}(t_i) - \frac{1}{F N_{1n}}\left[I_i(t - t_i) + \frac{1}{2}\frac{\left(I_f - I_i\right)}{\left(t_f - t_i\right)}(t - t_i)^2\right]. \tag{10}$$

Substituting $t = t_f$ and simplifying gives the average concentration of solid phase Li in the negative electrode at the final time as

$$\bar{C}_{1n}\left(t_f\right) = \bar{C}_{1n}(t_i) - \frac{1}{2}\frac{1}{F N_{1n}}\left(I_i + I_f\right)\left(t_f - t_i\right). \tag{11}$$

Using the condition, $I_i = I_f = I$ the above expression reduces to the solution for a constant current period.

According to the electro-neutrality condition, for every neutral Li ionized in an electrode, a Li + ion is neutralized in the opposite electrode. Thereby, the total number of neutral Li in the solid phase of both the electrodes remains constant (Eq. (128) in Ref. [4])

$$l_n \varepsilon_{1n} \bar{c}_{1n}(t) + l_p \varepsilon_{1p} \bar{c}_{1p}(t) = l_n \varepsilon_{1n} c_{1n0} + l_p \varepsilon_{1p} c_{1p0} = \text{Constant}. \tag{12}$$

In terms of scaled quantities, the above equation becomes

$$N_{1n}\bar{C}_{1n}(t) + N_{1p}\bar{C}_{1p}(t) = N_{1n}SoC_{n0} + N_{1p}SoC_{p0}, \tag{13}$$

where $N_{1p} = l_p \varepsilon_{1p} c_{sp\,max}. \tag{14}$

The initial condition is assumed to be a completely equilibrated state, that is, no concentration gradients or equivalently, the average concentration of Li within the active material spheres is equal to the surface concentration. Hence, the initial scaled concentrations are identical to initial electrode states of charge. Using the Eq. (13), the average Li concentration in the positive electrode is computed as

$$\bar{C}_{1p}(t) = SoC_{p0} + \frac{N_{1n}}{N_{1p}}\left[SoC_{n0} - \bar{C}_{1n}(t)\right]. \tag{15}$$

The average concentration gradient within the active material spheres in the negative electrode is scaled using maximum concentration and particle radius as

$$\bar{C}_{1rn} = \frac{r_n}{c_{sn\,max}}\bar{c}_{1rn}. \tag{16}$$

The evolution equation for the radial concentration gradient in negative electrode is given by (Eq. (153) in Ref. [4])

$$\frac{d\bar{c}_{1rn}}{dt} + \frac{30 D_{1n}}{r_n^2}\bar{c}_{1rn} = -\frac{45}{2r_n^2}\langle j_n \rangle. \tag{17}$$

With the solid diffusion time scale in negative electrode defined as

$$\tau_{1n} = \frac{r_n^2}{D_{1n}}. \tag{18}$$

Using Eqs. (2), (8), (16) and (18), Eq. (17) gets scaled as

$$\frac{d\bar{C}_{1rn}}{dt} + \frac{30}{\tau_{1n}}\bar{C}_{1rn} = -\frac{15}{2}\frac{1}{F N_{1n}}\left[I_i + \frac{\left(I_f - I_i\right)}{\left(t_f - t_i\right)}(t - t_i)\right]. \tag{19}$$

Eq. (19) is a first order differential equation which can be solved by more than one method. M. R. Spiegel [5] has details of such solution methods. In the present work, the equation is solved by obtaining the general solution which is the sum of a complementary function and a particular integral. The complementary function obtained by solving the homogeneous ODE, is

$$\overline{C}_{1rn}^{CF} = \alpha_n \exp\left[-30\frac{(t-t_i)}{\tau_{1n}}\right]. \tag{20}$$

To obtain the particular integral, a trial function linear in time is substituted in Eq. (19)

$$\overline{C}_{1rn}^{PI} = \beta_n + \gamma_n(t-t_i). \tag{21}$$

Equating the coefficients of the constant and the linear terms in time, in Eq. (21), the expressions for β_n and γ_n are obtained as,

$$\gamma_n = -\frac{1}{4}\frac{(I_f - I_i)\tau_{1n}}{FN_{1n}}\frac{1}{(t_f - t_i)}, \tag{22}$$

and $\beta_n = \frac{1}{4}\frac{I_i\tau_{1n}}{FN_{1n}} - \frac{1}{30}\gamma_n\tau_{1n}.$ \hfill (23)

The complete solution is the sum of complementary function and particular integral

$$\overline{C}_{1rn}(t) = \alpha_n \exp\left[-30\frac{(t-t_i)}{\tau_{1n}}\right] + \beta_n + \gamma_n(t-t_i). \tag{24}$$

At the initial time, the above expression reduces to

$$\overline{C}_{1rn}(t_i) = \alpha_n + \beta_n, \tag{25}$$

giving $\alpha_n = \overline{C}_{1rn}(t_i) - \beta_n.$ \hfill (26)

Thus, Eqs. (22), (23) and (26) determine the three coefficients in the complete solution of Eq. (24). For the initial condition of an equilibrated state, the initial average radial concentration gradient can be set to zero. Knowing the average concentration and the average radial concentration gradient, the negative electrode SoC is obtained by scaling Eq. (149) in Ref. [4] as,

$$SoC_n(t) = \frac{c_{sn}(t)}{c_{sn\,max}} = \overline{C}_{1n}(t) + \frac{8}{35}\overline{C}_{1nr}(t) - \frac{1}{105}\frac{I(t)\tau_{1n}}{FN_{1n}}. \tag{27}$$

Similarly, the average radial gradient in the positive electrode is obtained by solving the following equations (Eqs. (153) and (15) in Ref. [4])

$$\frac{d\overline{c}_{1rp}}{dt} + \frac{30D_{1p}}{r_p^2}\overline{c}_{1rp} = -\frac{45}{2r_p^2}\langle j_p \rangle, \tag{28}$$

where $\langle j_p \rangle(t) = -\frac{I(t)}{a_p Fl_p},$ \hfill (29)

and $a_p = \frac{3\varepsilon_{1p}}{r_p}.$ \hfill (30)

With the maximum solid phase Li capacity from Eq. (14) and the solid diffusion time constant

$$\tau_{1p} = \frac{r_p^2}{D_{1p}}, \tag{31}$$

Eq. (28) gets scaled as

$$\frac{d\overline{C}_{1rp}}{dt} + \frac{30}{\tau_{1p}}\overline{C}_{1rp} = \frac{15}{2}\frac{1}{N_{1p}F}\left[I_i + \frac{(I_f - I_i)}{(t_f - t_i)}(t-t_i).\right] \tag{32}$$

Its complete solution is obtained as

$$\overline{C}_{1rp}(t) = \alpha_p \exp\left[-\frac{30}{\tau_{1p}}(t-t_i)\right] + \beta_p + \gamma_p(t-t_i), \tag{33}$$

where $\gamma_p = \frac{1}{4}\frac{(I_f - I_i)\tau_{1p}}{FN_{1p}}\frac{1}{(t_f - t_i)},$ \hfill (34)

$$\beta_p = \frac{1}{4}\frac{I_i\tau_{1p}}{FN_{1p}} - \frac{1}{30}\gamma_p\tau_{1p}, \tag{35}$$

and $\alpha_p = \overline{C}_{1rp}(t_i) - \beta_p.$ \hfill (36)

Using the expressions for the average concentration and the average radial concentration gradient, the positive electrode SoC is obtained by scaling Eq. (149) in Ref. [4] as

$$SoC_p(t) = \frac{c_{sp}(t)}{c_{sp\,max}} = \overline{C}_{1p}(t) + \frac{8}{35}\overline{C}_{1pr}(t) + \frac{1}{105}\frac{I(t)\tau_{1p}}{FN_{1p}}. \tag{37}$$

2.2. Electrolyte phase Li concentration in the electrodes and the separator

The initial specific moles of Li, in the electrolyte phase of the electrode and separator regions, are defined as

$$N_{2k} = l_k\varepsilon_{2k}c_{20}, \tag{38}$$

and the electrolyte diffusion time constants $\tau_{2k} = \frac{l_k^2\varepsilon_{2k}}{D_{2k}},$ \hfill (39)

where $k = n, s, p$. It is to be noted that in Eq. (39), D_{2k} is the effective diffusivity that includes the effects of porosity and the Bruggeman factor. Details of the scaling are given in the 'Notation' section. The total specific moles of Li in the electrolyte phase of the cell is given by

$$N_2 = N_{2n} + N_{2s} + N_{2p}. \tag{40}$$

Electrolyte concentration field is characterized by the electrolyte flux at the two electrode−separator interfaces: $q_{2in}(t)$ and $q_{2ip}(t)$. The coupled ODEs for these two internal variables in ROM are (Eqs. (83) and (84) in Refs. [4], along with the average reaction rates Eqs. (2) and (5) herein)

$$a_{11}\frac{dq_{2in}}{dt} + a_{12}\frac{dq_{2ip}}{dt} = -q_{2in} + (1-t_+)\frac{I(t)}{F}, \tag{41}$$

and $a_{21}\frac{dq_{2in}}{dt} + a_{22}\frac{dq_{2ip}}{dt} = q_{2ip} - (1-t_+)\frac{I(t)}{F},$ \hfill (42)

where the coefficients (having units of time) in these ODEs are written in terms of the scaled quantities as

$$a_{11} = -\left(\frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s} + \frac{\tau_{2s}}{6} + \frac{\tau_{2n}}{3}\right)\frac{N_{2n}}{N_2} + \frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s} + \frac{\tau_{2n}}{3}, \tag{43}$$

$$a_{12} = -\left(\frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s} + \frac{\tau_{2s}}{3} - \frac{\tau_{2p}}{3}\right)\frac{N_{2n}}{N_2} + \frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s}, \tag{44}$$

$$a_{21} = -\left(\frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s} + \frac{\tau_{2s}}{6} + \frac{\tau_{2n}}{3}\right)\frac{N_{2p}}{N_2}, \tag{45}$$

and $a_{22} = -\left(\frac{1}{2}\frac{N_{2n}}{N_{2s}}\tau_{2s} + \frac{\tau_{2s}}{3} - \frac{\tau_{2p}}{3}\right)\frac{N_{2p}}{N_2} - \frac{\tau_{2p}}{3}.$ \hfill (46)

Rearranging Eq. (41) gives

$$\frac{dq_{2ip}}{dt} = -\frac{1}{a_{12}}q_{2in} - \frac{a_{11}}{a_{12}}\frac{dq_{2in}}{dt} + \frac{1}{a_{12}}\frac{(1-t_+)}{F}I(t). \tag{47}$$

Using this equation in Eq. (42) and rearranging gives

$$q_{2ip} = -\frac{a_{22}}{a_{12}}q_{2in} - \frac{deta}{a_{12}}\frac{dq_{2in}}{dt} + \left(\frac{a_{22}}{a_{12}} + 1\right)\frac{(1-t_+)}{F}I(t). \tag{48}$$

Differentiating the above equation with respect to time, and using the current profile of Eq. (8) gives

$$\frac{dq_{2ip}}{dt} = -\frac{a_{22}}{a_{12}}\frac{dq_{2in}}{dt} - \frac{deta}{a_{12}}\frac{d^2q_{2in}}{dt^2} + \left(\frac{a_{22}}{a_{12}} + 1\right)\frac{(1-t_+)}{F}\left(\frac{I_f - I_i}{t_f - t_i}\right). \tag{49}$$

Using the above equation coupled with Eq. (8) in Eq. (41) followed by simplification gives

$$deta\frac{d^2q_{2in}}{dt^2} - (a_{11} - a_{22})\frac{dq_{2in}}{dt} - q_{2in}$$
$$= -\frac{(1-t_+)}{F}\left[I_i + \frac{(I_f - I_i)}{(t_f - t_i)}(t - t_i - a_{12} - a_{22})\right]. \tag{50}$$

This equation is a second order ODE with a time-dependent forcing function. Its complementary function is obtained from the homogeneous part of the ODE as follows: Solving the quadratic equation

$$deta\lambda^2 - (a_{11} - a_{22})\lambda - 1 = 0, \tag{51}$$

gives the roots λ_1 and λ_2. Then, the complementary function is

$$q_{2in}^{CF}(t) = A\exp(\lambda_1 t) + B\exp(\lambda_2 t). \tag{52}$$

The particular integral is obtained as follows: Substituting the linear trial function

$$q_{2in}^{PI}(t) = P + Qt, \tag{53}$$

in the ODE Eq. (50) and simplifying gives

$$(a_{11} - a_{22})Q + (P + Qt) = \frac{(1-t_+)}{F}\left[I_i + \frac{(I_f - I_i)}{(t_f - t_i)}(t - t_i - a_{12} - a_{22})\right]. \tag{54}$$

Equating the coefficients of the linear and constant terms in time gives

$$Q = \frac{(1-t_+)}{F}\frac{(I_f - I_i)}{(t_f - t_i)}, \tag{55}$$

and, $$P = \frac{(1-t_+)}{F}I_i - (t_i + a_{11} + a_{12})Q. \tag{56}$$

The complete solution to the ODE Eq. (50) is the sum of the complementary function Eq. (52) and the particular integral Eq. (53)

$$q_{2in}(t) = A\exp(\lambda_1 t) + B\exp(\lambda_2 t) + P + Qt. \tag{57}$$

With P and Q determined from Eqs. (55) and (56), A and B are

determined from the initial value and the initial rate of change of q_{2in}, as shown below. Differentiating Eq. (57) gives

$$\frac{dq_{2in}}{dt} = A\lambda_1 \exp(\lambda_1 t) + B\lambda_2 \exp(\lambda_2 t) + Q. \tag{58}$$

Using Eqs. (57) and (58) in Eq. (48) and simplifying gives

$$q_{2ip} = -\frac{1}{a_{12}}(a_{22} + deta\lambda_1)A\exp(\lambda_1 t) - \frac{1}{a_{12}}(a_{22} + deta\lambda_2)B\exp(\lambda_2 t) - \frac{a_{22}}{a_{12}}(P + Qt) - \frac{deta}{a_{12}}Q + \left(\frac{a_{22}}{a_{12}} + 1\right)\frac{(1-t_+)}{F}I(t). \tag{59}$$

The initial values of q_{2in} and q_{2ip} are set to zero at the beginning of the simulation based on the assumption of equilibrated state. At successive time intervals they are obtained by their continuity in time i.e. their values at the end of the previous time interval are the initial values for the successive time interval. Once the initial values of q_{2in} and q_{2ip} are known, the coefficients A and B can be obtained by solving Eqs. (57) and (59).

3. Algebraic ROM algorithm

In this section an explicit algebraic reduced order algorithm is constructed using the theoretical results collated in Section 7 of [4] and those derived in the earlier section of this work. The initial state is assumed to be equilibrated i.e. the cell is rested until the concentration gradients in the electrolyte and solid phases have relaxed. The steps in the algorithm are:

1. Computation of average concentration based SoC in negative electrode: Eq. (10).
2. Computation of average radial gradient in negative electrode: Eq. (24).
3. Computation of SoC in negative electrode: Eq. (27).
4. Computation of average concentration based SoC in positive electrode using solid Li balance: Eq. (15).
5. Computation of average radial gradient in positive electrode: Eq. (33).
6. Computation of SoC in positive electrode: Eq. (37).
7. Computation of interfacial electrolyte fluxes: Eqs. (57) and (59).
8. Computation of interfacial, average, collector-end and mid-separator electrolyte concentrations using interfacial fluxes: Eqs. (77), (78), (57), (74), (65), (60), (67), (76) of [4].
9. Computation of interfacial and collector-end electrolyte potentials: Eqs. (105), (106), (114) and (117) of [4].
10. Computation of collector-end solid potentials and hence the cell voltage: Eqs. (157) and (158) of [4].

This algorithm is used to compare the algebraic ROM prediction with the Matlab–Simulink result of the original ROM of [4] for a constant current discharge case in Fig. 1. This figure shows that the order reduction to algebraic level is indeed exact at both nominal and high current discharge rates.

4. Conclusions

Real-time voltage prediction of lithium ion cells using the electrochemical model is difficult owing to solving coupled partial differential equations. In an earlier publication [4] a reduced order model (ROM) was developed by reducing the partial differential
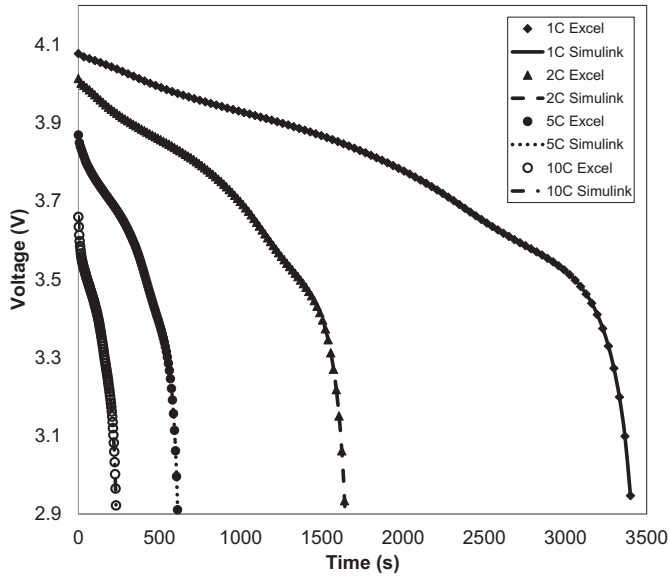
Fig. 1. Comparison of Excel implementation of algebraic ROM with the Simulink implementation of ODEs based ROM for constant current discharge at various discharge rates.

equations to a set of five linear ordinary differential equations and nonlinear algebraic expressions. This is achieved [4] by applying order reduction methodologies such as uniform reaction rate approximation, volume averaging and profile based approximations. In the present work, this model reduction approach is applied for any arbitrary current profile. An arbitrary current profile, involving charge, rest and discharge, is expressed as a series of constant current and linearly varying current periods. The latter is more generic, since it includes the constant current period as well. The linear ordinary differential equations in ROM are solved using the analytical form of the linearly varying current and an explicit algebraic algorithm is developed for lithium ion cell voltage prediction. Owing to the simplicity of the algorithm, it is amenable for implementation on spreadsheets which can be used to validate laboratory test data and can be extended to a battery management system for onboard application in electric vehicles and smartphones.

References

[1] M. Doyle, J. Newman, J. Electrochem. Soc. 143 (1996) 1890–1903.
[2] V.R. Subramanian, V. Boovaragavan, V.D. Diwakar, Electrochem. Solid-State Lett. 10 (2007) A255–A260.
[3] V.R. Subramanian, V.D. Diwakar, D. Tapriyal, J. Electrochem. Soc. 152 (2005) A2002–A2008.
[4] V. Senthil Kumar, J. Power Sources 222 (2013) 426–441.
[5] M.R. Spiegel, Theory and Problems of Advanced Mathematics for Engineers and Scientists, Schaum's Outline Series, McGraw-Hill Inc., 1971 edition, 24th printing 1996.

Notation

Constants & variables
R: Gas constant, 8.314 J mol^{-1} K^{-1}.
F: Faraday's constant, 96487 C mol^{-1}.
T: Temperature, 298 K in this work.
$I(t)$: External current density at time t, A m^{-2}.
I_i, I_f: External current densities at times t_i and t_f in a linearly varying current pulse, A m^{-2}.
t_+: Electrolyte transference number, dimensionless.
brug: Bruggeman factor, used to calculate effective porous media properties, dimensionless.
l_n, l_s, l_p: Thickness of negative electrode, separator and positive electrode, m. $L = l_n + l_s + l_p$ is total cell thickness.
r_n, r_p: Radii of active material spheres in the negative and positive electrodes, m.
$\varepsilon_{1k}, \varepsilon_{2k}, \varepsilon_{fk}$: Volume fractions of active material, electrolyte and filler in electrode or separator domains, dimensionless. $\varepsilon_{1k} + \varepsilon_{2k} + \varepsilon_{fk} = 1$. Separator has no active material. Hence $\varepsilon_{1s} = 0$.
$a_k = 3\varepsilon_{1k}/r_k$: Specific surface area of active materials in n and p electrodes, m^{-1}.
j_k: Local surface reaction rate in $k = n, p$ electrodes, mol m^{-2}s^{-1}.
$j_{k0} = k_k(c_{sk\,max} - c_{sk})^{0.5}c_{sk}^{0.5}c_2^{0.5}$: Over-potential independent rate pre-factor, mol m^{-2} s^{-1}.
k_k: Surface reaction rate constant in $k = n, p$ electrodes, (mol m^{-2} s^{-1})(mol m^{-3})$^{-1.5}$.
c_1, c_2: Solid phase concentration in active material spheres and electrolyte concentration, mol m^{-3}.
$c_{sk}, c_{sk\,max}$: Surface solid phase concentrations, and their maximum value, mol m^{-3}.
$\overline{C}_{1k} = \overline{c}_{1k}/c_{sk\,max}$: Scaled average solid phase concentrations in $k = n, p$ electrodes, dimensionless.
$\overline{C}_{1rk} = r_k\overline{c}_{1rk}/c_{sk\,max}$: Scaled average radial gradient in $k = n, p$ electrodes, dimensionless.
c_{2ik}, q_{2ik}: Interfacial electrolyte concentraions and fluxes, mol m^3, mol m^{-2} s^{-1}.
D_2: Electrolyte diffusivity (material property), m^2 s^{-1}.
$D_{2k} = D_2 \times \varepsilon_{2k}^{brug}$: Effective electrolyte diffusivity in the porous $k = n, s, p$ domains.
D_{1k}: Solid diffusivity of $k = n, p$ electrode material spheres, m^2 s^{-1}.
κ_2: Electrolyte conductivity (material property), S m^{-1}.
$\kappa_{2k} = \kappa_2 \times \varepsilon_{2k}^{brug}$: Effective electrolyte conductivity in porous $k = n, s, p$ domains.
N_{1k}: Maximum specific moles of solid Li in $k = n, p$ electrodes, mol m^{-2}.
N_{2k}: Initial specific moles of electrolyte Li in $k = n, s, p$ regions, mol m^{-2}.
$N_2 = N_{2n} + N_{2s} + N_{2p}$: Total molar capacity of electrolyte Li in the cell, mol m^{-2}.
σ_k: Electrical conductivity of $k = n, p$ electrode materials (material property), S m^{-1}
$\sigma_{1k} = \sigma_k \times \varepsilon_{1k}^{brug}$: Effective electrical conductivity in the porous $k = n, p$ domains, S m^{-1}.
Φ_1, Φ_2: Solid and liquid potential, V.
τ_{1k}: Solid diffusion time constants in $k = n, p$ electrodes.
τ_{2k}: Electrolyte diffusion time constants in $k = n, s, p$ domains.
U_k: Open circuit voltage of $k = n, p$ electrodes, V.
$SoC_k = c_{sk}/c_{s\,max\,k}$: State of charge of $k = n, p$ electrodes, dimensionless.

Subscripts and operators:
1, 2, f: Solid active material, liquid electrolyte phases and solid fillers (including additives)
$k = n, s, p$: Negative electrode, separator, and positive electrode.
in: Separator interface of the negative electrode.
ip: Separator interface of the positive electrode.
CF: Complementary function of an ordinary differential equation.
PI: Particular integral of an ordinary differential equation.
0: Initial condition.
r: Radial gradient.
$\langle \cdot \rangle$: Volume average, defined in the three domains, n, s, p.
$\overline{\cdot}$: Volume average within an active material sphere in n or p electrode.